1-[(1H-Benzotriazol-L-yl)methyl]pyridinium

Inchi: InChI=1S/C12H11N4/c1-4-8-15(9-5-1)10-16-12-7-3-2-6-11(12)13-14-16/h1-9H,10H2/q+1
InchiKey: NEMINUYEACMXFA-UHFFFAOYSA-N
Formula: C12H11N4
SMILES: c1cc[n+](Cn2nnc3ccccc32)cc1
Mol. weight [g/mol]: 211.24
CAS: 125713-96-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	1.225		Crippen Method
mcvol	159.330	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C125713964&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume